

Species Tag:	42006	Species Name:	C-13-H3CN
Version:	1		Acetonitrile,
Date:	April 1996		¹³ C on methyl isotope
Contributor:	J. C. Pearson		

Lines Listed:	9015	Q(300.0)=	31255.7307
Freq. (GHz) <	1773	Q(225.0)=	20296.6968
Max. J:	99	Q(150.0)=	11047.3940
LOGSTR0=	-10.0	Q(75.00)=	3908.0709
LOGSTR1=	-10.0	Q(37.50)=	1387.1037
Isotope Corr.:	-1.955	Q(18.75)=	507.4819
Egy. (cm ⁻¹) >	0.0	Q(9.375)=	197.9113
μ_a =	3.92197(13)	A=	158107.7
μ_b =		B=	8933.3
μ_c =		C=	B

The experimental measurements are from: D. Boucher, J. Burie, A. Bauer, A. Dubrulle and J. Demaison, 1980, J. Phys. Chem. Ref. Data **9**, 659., J. C. Pearson and H. S. P. Müller, 1996, Astrophys J. Lett., submitted., and B. Gatehouse and T. Brupbacher, 1996, private communication.

The details of the analysis are presented in the Pearson and Müller paper. The constants A, D_K, H_K cannot be determined from the microwave spectra and were determined by scaling the IR measurements of: R. Anttila, V.-M. Horneman, M. Koivussaari and R. Paso, 1993, J. Mol. Spect. **157**, 198, and M. Koivussaari, V.-M. Horneman and R. Anttila, 1992, J. Mol. Spect. **152**, 377 by the ground state average (r_z) structure differences from normal species. Other higher order constants (H_J, L_{JJK}, L_{JK}, L_{KKJ}) were fixed to scaled from the normal species (tag 41001).

The dipole moment was fixed to the main isotope reported by J. Gadhi, A. Lahrouni, J. Legrand, and J. Demaison, 1995, J. Chem. Phys. **92**, 1984.